CLAIMS

We claim:

1. A molecule or molecular complex comprising all or any parts of a binding pocket defined by structure coordinates of IMPDH amino acids 68, 69, 93, 273, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 330, 331, 332, 333, 334, 337, 339, 340, 364, 413, 414, 415, 416, 420, 439, 440, 441, 442, 469, and 470 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

2. The molecule or molecular complex according to claim 1, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 274, 275, 276, 277, 303, 322, 324, 325, 326, 331, 333, 414, 415, and 441 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

3. The molecule or molecular complex according to claim 2, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 275, 276, 303, 325, 326, 331, 333 and 441 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

4. A molecule or molecular complex comprising all or any parts of a binding pocket defined by structure coordinates of IMPDH amino acids 67, 68, 69, 70, 73, 274, 275, 276, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 440, 441, 442, 443, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

5. The molecule or molecular complex according to claim 4, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 68, 69, 70, 303, 322, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 419, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

6. The molecule or molecular complex according to claim 5, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 68, 70, 322, 328, 329, 331, 332, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root

mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

7. The molecule or molecular complex according to claim 4, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 67, 68, 69, 70, 73, 93, 273, 274, 275, 276, 277, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 337, 339, 340, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 420, 439, 440, 441, 442, 443, 469, 470, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

8. The molecule or molecular complex according to claim 7, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 68, 69, 70, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

9. The molecule or molecular complex according to claim 8, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 68, 70, 275,

276, 303, 322, 325, 326, 328, 329, 331, 332, 333, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

10. The molecule or molecular complex according to claim 7, wherein said molecule or molecular complex is defined by the set of structure coordinates according to Figure 1, or a homologue thereof, wherein said homologue has a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å.

11. The molecule or molecular complex according to claim 7, wherein said molecule or molecular complex comprises amino acids 1-514 of IMPDH, XMP*, and MPA.

12. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex comprising all or any parts of a binding pocket defined by structure coordinates of IMPDH amino acids 68, 69, 93, 273, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 330, 331, 332, 333, 334, 337, 339, 340, 364, 413, 414, 415, 416, 420, 439, 440, 441, 442, 469, and 470 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square

deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

13. The machine-readable data storage medium according to claim 12, wherein said binding pocket defined by structure coordinates of IMPDH amino acids 274, 275, 276, 277, 303, 322, 324, 325, 326, 331, 333, 414, 415, and 441 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

14. The machine-readable data storage medium according to claim 13, wherein said binding pocket defined by structure coordinates of IMPDH amino acids 275, 276, 303, 325, 326, 331, 333 and 441 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

15. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of all or any parts of a molecule or molecular complex comprising a binding pocket defined by structure coordinates of IMPDH amino acids 67, 68, 69, 70, 73, 274, 275, 276, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 364, 365, 366, 367, 368, 385, 386, 387, 388,

389, 391, 411, 412, 413, 414, 415, 416, 419, 440, 441, 442, 443, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

16. The machine-readable data storage medium according to claim 15, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 68, 69, 70, 303, 322, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 419, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

17. The machine-readable data storage medium according to claim 16, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 68, 70, 322, 328, 329, 331, 332, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

18. The machine-readable data storage medium according to claim 15, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 67,

68, 69, 70, 73, 93, 273, 274, 275, 276, 277, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 337, 339, 340, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 420, 439, 440, 441, 442, 443, 469, 470, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

19. The machine-readable storage medium according to claim 18, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 68, 69, 70, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

20. The machine-readable storage medium according to claim 19, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 68, 70, 275, 276, 303, 322, 325, 326, 328, 329, 331, 332, 333, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than

1.5 Å.

21. The machine-readable data storage medium, according to claim 18, wherein said molecule or molecular complex is defined by the set of structure coordinates for IMPDH according to Figure 1, or a homologue of said molecule or molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

22. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates for IMPDH according to Figure 1; and said second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex of unknown structure.

23. A method for evaluating the ability of a chemical entity to associate with a molecule or molecular complex according to any one of claims 1 to 11 comprising the steps of:

a. employing computational means to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex; and

b. analyzing the results of said fitting

operation to quantify the association between the chemical entity and the binding pocket.

24. A method of utilizing molecular replacement to obtain structural information about a molecule or a molecular complex of unknown structure by using the structure coordinates set forth in Figure 1, comprising the steps of:

a. crystallizing said molecule or molecular complex;

b. generating an X-ray diffraction pattern from said crystallized molecule or molecular complex;

c. applying at least a portion of the structure coordinates set forth in Figure 1 to the X-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

25. The method according to claim 24, wherein the molecule or molecular complex comprises a polypeptide selected from an IMPDH homologue.

26. A method for preparing a IMPDH/XMP*/MPA crystal comprising the steps of:

a. forming a complex between IMPDH and IMP;

b. adding NAD and MPA to the complex formed in step a;

c. monitoring the accumulation of the IMPDH/XMP*/MPA complex; and

d. crystallizing the complex formed in step c in the presence of MeP.

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